# Electronic Structure of $URu_2Si_2$

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## INTRODUCTION

Heavy fermion compounds are characterized by a large linear specific heat coefficient ($\gamma$) which signals large ('heavy') effective masses of electrons forming the Fermi surface. $URu_2Si_2$, which has a moderately large linear specific heat coefficient of $\gamma$~180 mJ/mol-$K^2$ [1] extrapolated from the paramagnetic phase (T>17.5 K). Previous ARPES experiments on $URu_2Si_2$ have (a) determined the crystal inner potential ($V_0$~12 eV), (b) mapped the basic *d*-band structure along high symmetry directions and (c) established the existence of hole pockets at the $\Gamma$, Z and X-points of the Brillouin zone [2-4]. The focus of this abstract is to present a detailed comparisonof the experimental valence bandstructure to theoretical LDA calculations and to rationalize the observed the large near-$E_F$ discrepancies.

## EXPERIMENT

$URu_2Si_2$ has the $ThCr_2Si_2$ crystal structure with a body-centered tetragonal Brillouin zone. Single crystal samples were cleaved in ultra-high vacuum ($<1.2\times10^{-10}$ torr) at room temperature exposing the [001] surface and then cooled to ~150 K for ARPES measurements at ALS Beamline 7.0.1.2. The Fermi-edge intensity mapping technique using automated angular motions was employed to gain an overview of the sample orientation and Fermi surface structure. A total instrumental resolution of ≈80 meV and full angular acceptance of ≈0.7° was employed. Additional ARPES experiments focused on the ***k***-dependent U 5*f* spectral weight, not discussed here, were performed at $5d\rightarrow4f$ resonant photon energies (98 and 108 eV)

## RESULTS

Fig. 1(a) presents reverse grayscale images of $URu_2Si_2$ valence band spectra along two high-symmetry azimuths at two different off-resonance photon energies. The residual *f*-weight far above-resonance at 156 eV is evident near $E_F$ in contrast to the near complete suppression of f-weight and strong *d*-cross section below 1.5 eV observed for the 85 eV data. Comparison to the other $XRu_2Si_2$ band structures and to the LDA calculations in Fig. 1(b) show the common features of parabolic-like band dispersions with band minima at ≈1.6 eV binding energy centered around the X-point and midway between $\Gamma$ and Z. Also at the Z-point, band maxima at ≈0.5 eV and ≈0 eV are observed in agreement with bands (1,2) and 3, respectively, in the LDA calculation. Spectral intensity near $E_F$ just adjacent to the Z-point along Z-($\Sigma$)-$\Gamma$ has a possible correspondence to bands 4 and/or 5.

In contrast to the other $XRu_2Si_2$ systems, the experimental bands in Fig. 1(a) also reveal quite strong disagreements with the LDA calculation in the near-$E_F$ region where experimental dispersions down to below 1 eV have no correspondence to theory. At 156 eV, the $\Gamma$-($\Sigma$)-Z data show a strong electron-like dispersion centered on $\Gamma$ that crosses $E_F$ close to the midpoint between $\Gamma$ and

Z. This band dispersion can be traced all the way to ≈1.5 eV binding energy at the Γ-point. Its presence is also evident at lower photon energies with weaker relative intensity and it serves as an additional signature that distinguishes the Γ and Z points. Along Γ-X-Γ, a data set from 85 eV is chosen to highlight a second anomaly relative to the LDA calculation, i.e. the presence of a distinct hole pocket centered on the "X"-point. This band dispersion can be traced to below 0.5 eV and has no clear theoretical counterpart in the $URu_2Si_2$ band calculations that predict the possible presence of a small electron-like pocket arising from a shallow dispersing band of f-character that dips below $E_F$.

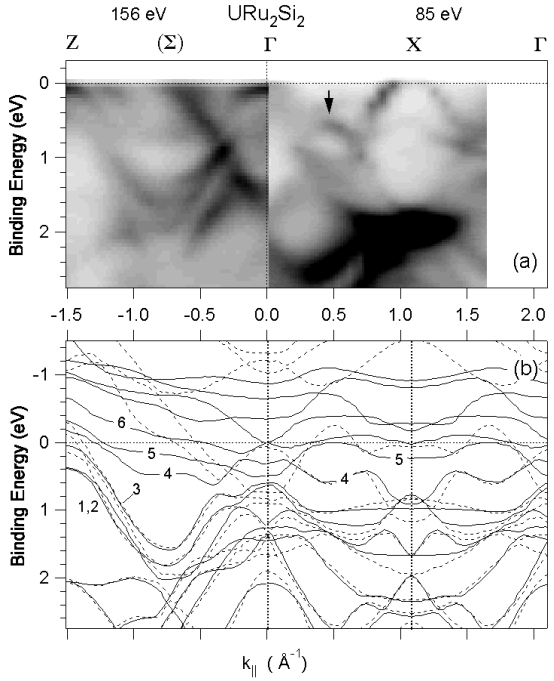


Figure 1. (a) Valence band intensity maps of $URu_2Si_2$ at 156 and 85 eV along high-symmetry azimuth angles corresponding to Γ–(Σ)–"Z" and Γ–X–"Γ". (b) Theoretical band structure calculation for $URu_2Si_2$ (solid) and $ThRu_2Si_2$ (dashed).

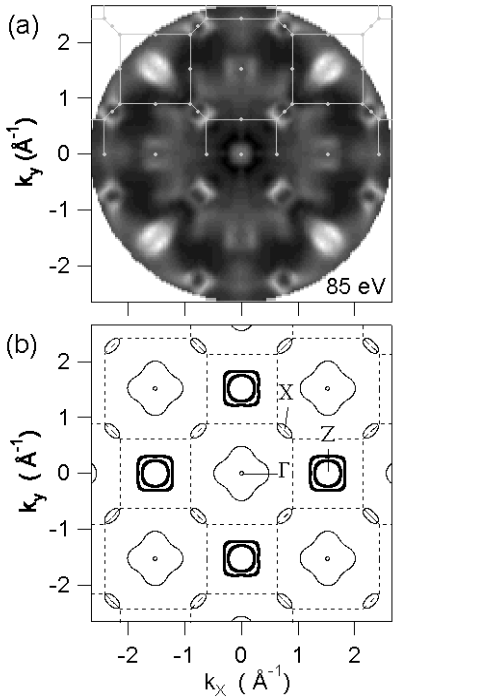


Figure 2. (a) Off-resonance Fermi-energy intensity maps of $URu_2Si_2$ at 85eV. (c) Theoretical contours of hole (bold) and electron (fine) Fermi surface topologies.

Another view of this "X"-point discrepancy is in the comparison of an experimental $E_F$ intensity map at 85 eV in Fig. 2(a), with the theoretical FS contours in Fig. 2(b). The off-resonance FS map was acquired over a 80° azimuth range and 35° polar angle and has been 4-fold symmetrized. It exhibits intensity maxima surrounding the high symmetry $k_{||}$ locations suggestive of closed FS contours. Since the actual hemispherical measurement surface probes midway between Z and Γ along normal emission, a bct BZ centered on Z is overplotted on the FS map to reflect the fact that the measurement surface cuts close to Γ along <100> and close to Z along <110> in the second BZ's. At $k_{||}$ corresponding to the X-points, a squarish closed contour is nicely observed to additionally repeat near the outer edge of the FS map at the boundary between the second and third radial BZ's. All three of these relatively small FS contours at Γ, Z, and X originate from hole-like dispersions as shown in Fig. 1. In contrast, the theoretical FS contours in Fig. 2(b) show significantly larger hole pockets at the Γ-point and small electron pockets at the X-point.

## ANALYSIS

A major source of these large discrepancies with LDA is the well-known theoretical over-estimation of the 5*f* bandwidth which produces *f*-bands that disperse too strongly and cause unrealistic disruptions of the *d*-band FS. With this concept in mind we try to deduce the origin of the $URu_2Si_2$ X-point hole-pocket by comparing the experimental bands in Fig. 1(a) to $5f^0$ $ThRu_2Si_2$ bands (dashed lines) in Fig. 1(b). The dispersions of bands 4 and 5 near X appear to originate from the crossing-point hybridization between a parabolic electron-like band of Th *d*-character and a hole-like band of Ru *d*-character, both symmetric about the X-point. The resulting gap at the crossing point (≈0.3 eV) splits the two bands into two branches with the upper branch being band 5 near X. We then speculate that for $URu_2Si_2$, the presence of U 5*f* states, in addition to creating a very narrow band of states just above $E_F$, pushes the U-*d* electron-like band to lower energy (perhaps completely below $E_F$ with correspondence to the arrow in Fig. 1(a)). The result is that the U-*d* and Ru-*d* crossing point is also moved to lower energy, thereby allowing the X-point Ru-*d* hole-pocket to remain as the unhybridized continuation of band 4 above $E_F$.

Similarly, and perhaps more simply, a possible correspondence can be made between the anomalous electron-like dispersion centered at Γ in $URu_2Si_2$, which is particularly strong at 156 eV along Γ-(Σ)-Z, and bands 4 and/or 5 in the $5f^0$ LDA band structure of $ThRu_2Si_2$.

## REFERENCES


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